Supporting Information

Structure, dynamics and stability of water/scCO$_2$/mineral interfaces from ab initio molecular dynamics simulations

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S1. Simulation cell and structure of H_2O and CO_2 monolayers.

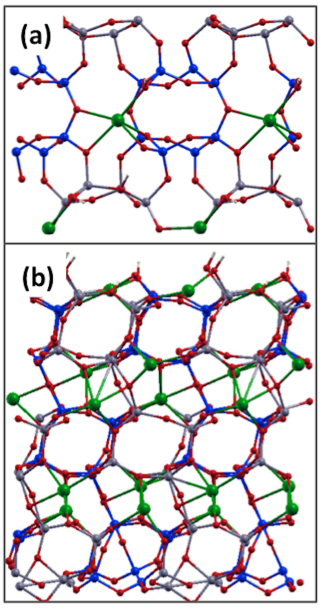

Figure 1. Structure of the Anorthite (001) slab used in this study: Atoms are represented by balls with color: Blue (Si), Grey (Al), Red (O), White (H) Green (Ca).

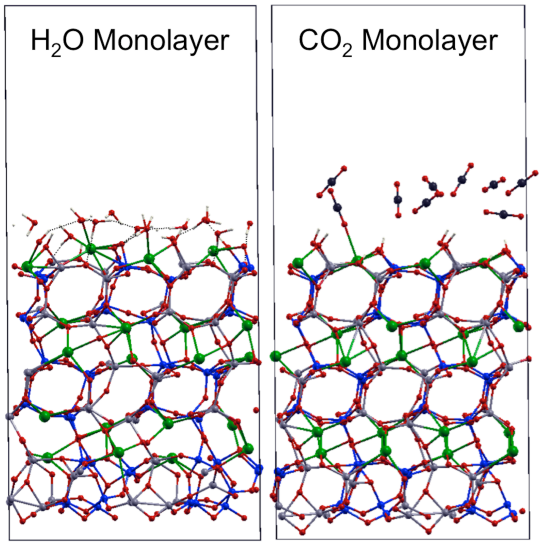

Figure 2. Structure of full coverage water and $scCO_2$ adlayer on the Ca-rich Anorthite (001) adlayer: H (white), C (black), O (red), Si (blue), Al (gray), and Ca (green).

S2. Summary of simulation cell parameters and validation of liquid state of water and scCO$_2$ layers from AIMD simulations.

Table 1. Optimized cell parameters and simulation time.

System	Cell parameters	Interlayer spacing (Å)	Simulation time (ps)
32CO$_2$	*a*=16.42 Å, *b*=13.10 Å, *c*=34.64 Å *α*=90.1º, *β*=90.5º, *γ*=91.6º	18.3	15
14H$_2$O	*a*=16.43 Å, *b*=13.07 Å, *c*=34.97 Å *α*=90.0º, *β*=90.5º, *γ*=91.4º	18.3	15
1H$_2$O/32CO$_2$	*a*=16.42 Å, *b*=13.10 Å, *c*=34.64 Å *α*=90.1º, *β*=90.5º, *γ*=91.6º	18.3	225*
2H$_2$O/31CO$_2$	*a*=16.42 Å, *b*=13.10 Å, *c*=34.64 Å *α*=90.1º, *β*=90.5º, *γ*=91.6º	18.3	224*
3H$_2$O/30CO$_2$	*a*=16.42 Å, *b*=13.10 Å, *c*=34.64 Å *α*=90.1º, *β*=90.5º, *γ*=91.6º	18.3	241*
10H$_2$O/28CO$_2$	*a*=16.41 Å, *b*=13.07 Å, *c*=33.25 Å *α*=89.9º, *β*=90.6º, *γ*=91.5º	17.0	294*
14H$_2$O/28CO$_2$	*a*=16.43 Å, *b*=13.07 Å, *c*=34.97 Å *α*=90.0º, *β*=90.5º, *γ*=91.4º	18.3	428*,†
15H$_2$O/28CO$_2$	*a*=16.43 Å, *b*=13.07 Å, *c*=34.97 Å *α*=90.0º, *β*=90.5º, *γ*=91.4º	18.3	246*
28H$_2$O/21CO$_2$	*a*=16.43 Å, *b*=13.07 Å, *c*=35.09 Å *α*=90.1º, *β*=90.6º, *γ*=91.3º	18.5	234*
42H$_2$O/20CO$_2$	*a*=16.42 Å, *b*=13.07 Å, *c*=36.12 Å *α*=90.1º, *β*=90.5º, *γ*=91.2º	19.2	28
84H$_2$O	*a*=16.39 Å, *b*=13.07 Å, *c*=36.07 Å *α*=90.2º, *β*=90.5º, *γ*=91.1º	19.3	20

* Total time for both constraint and unconstraint MD simulations.

† Simulations for Ca positions and CO_3 formation are also included.

Table 2. Summary of simulation cell parameters and validation of liquid state of water and $scCO_2$ layers from AIMD simulations.

Trajectory	Diffusion Coefficient[a] ($10^{-4}cm^2/s$)	Density[b] (g/cm^3)
$scCO_2$	1st layer: D_{xy}=0.3, D_z=0.2 Liquid: D_{xy}=1.4, D_z=0.4	1st layer: 1.2 Liquid: 0.40
Water	1st layer: D_{xy}=0.02, D_z=0.01 Liquid: D_{xy}=1.0, D_z=0.2	1st layer: 1.9 Liquid: 1.02
1W	1st layer: D_{xy}=0.03, D_z=0.01	1st layer: 2.1
1W/$scCO_2$	1st layer: D_{xy}=0.01, D_z=0.01 CO_2 Layer: D_{xy}=1.1, D_z=0.9 CO_2 Liquid: D_{xy}=1.0, D_z=0.3	1st layer: 1.9 CO_2 Layer: 0.84 CO_2 Liquid: 0.49
2W/$scCO_2$	1st layer: D_{xy}=0.02, D_z=0.01 CO_2 Liquid: D_{xy}=1.0, D_z=0.3	1st layer: 1.8 CO_2 Liquid: 0.29
3W/$scCO_2$	1st layer: D_{xy}=0.02, D_z=0.01 CO_2 Liquid: D_{xy}=1.0, D_z=0.3	1st layer: 1.9 CO_2 Liquid: 0.39

[a]Diffusion Coefficient of $scCO_2$ $5.2x10^{-4}cm^2/s$ (P=101bar,T=323K)[1] , H_2O $0.35x10^{-4}cm^2/s$ (P=101 bar, T=3218)[2]. [b]Density of $scCO_2$, $0.4g/cm^3$, H_2O $1.02g/cm^3$ (T=323K, P=100bar).

The computed values of the diffusion coefficient (D) and Density for water and CO_2 are given in **Supplementary Table 2**. The D values were extracted from the slope of the mean square displacement correlation function and decomposed into components that are parallel, D_{xy}, and perpendicular, D_z, to the surface, see **Supplementary Figure 3** for the 1W/$scCO_2$ case. In both cases the density and diffusion are satisfactorily comparable to values measured experimentally.

[1] P. Etesse, J. A. Zega, and R. Kobayashi, J. Chem. Phys. 97, 2022 (1992).
[2] Harris, Kenneth R., and Lawrence A. Woolf. *J. Chem. Soc., Faraday Transactions 1:* 76 (1980): 377-385.

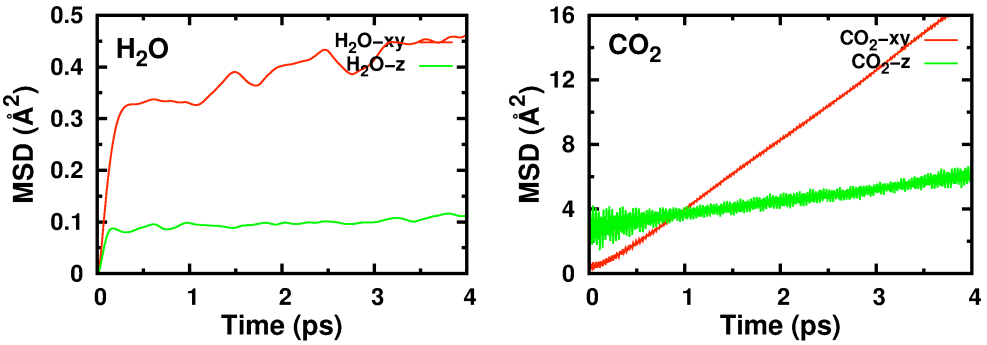

Figure 3. MSD for AIMD trajectory of H_2O (left) and $scCO_2$ (right) for $1W/scCO_2$ layer.

S3. Atomic density profiles following Ca dissolution.

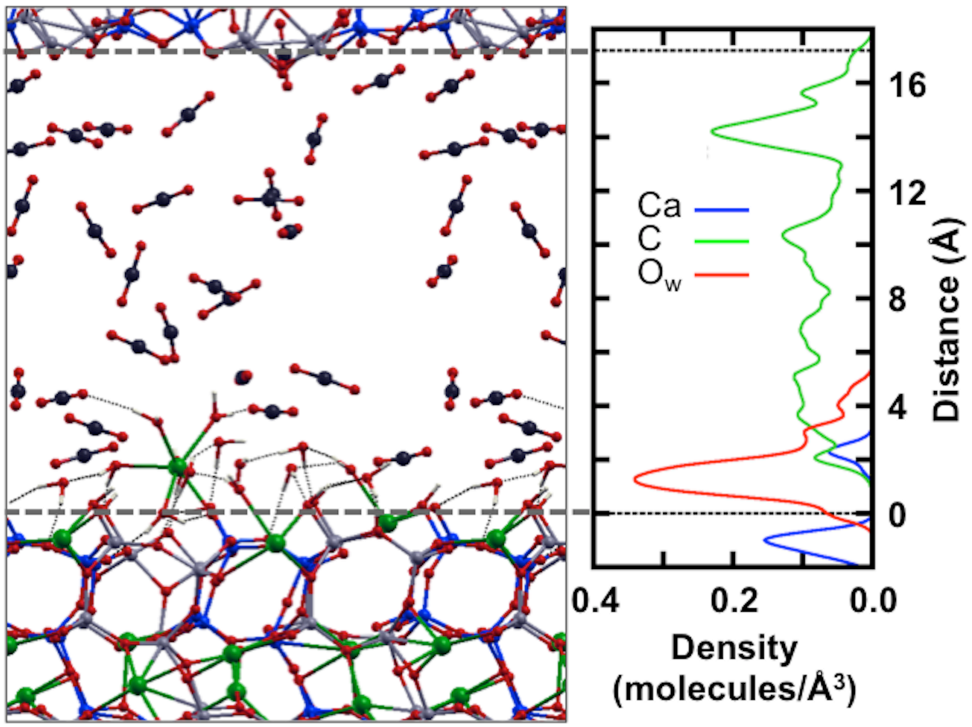

Figure 4. (a) Snapshot of liquid phases from AIMD runs at 323 K with Ca^{2+} ion solvated in 1W layer, Hydrogen (white), Carbon (dark grey), Oxygen (red), Silicon (blue), Aluminum (silver), Calcium (green). (b) Molecular density projected along the direction of the surface normal, Red (water), Green (CO_2), Blue (Ca).

S4. Convergence of PMF.

To calculate potential mean force (PMF), we employed constrained MD based on the Blue-Moon sampling method: at each point in the PMF (11-18 points) a short (~10 ps) simulation was performed. In **Supplementary Figure 5,** we plot the expectation value of our constrained force, <F>, as a function of our reaction distance, z coordinate of O_w, for selected PMFs. Error bars on <F> are estimated to be at most ±0.0004 a.u. As a rough estimate, an average bin with width of 0.4 Å gives an approximate error for each point in our integration of *ca* ±2 kJ/mol. A more detailed error analysis in the numerical integration of the force functions suggest an overall convergence of ±2kJ/mol for the ΔA values reported in the text.

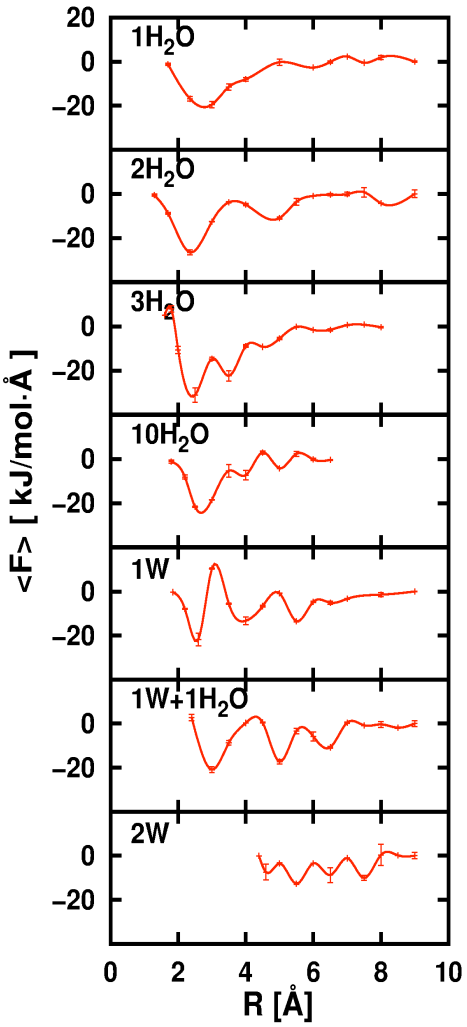

Figure 5. Expectation value of constrained force <F> in kJ/mol·Å. as a function of reaction distance. Error bars are estimated via a plateau analysis[1].

S5. Density profiles from selected PMFs

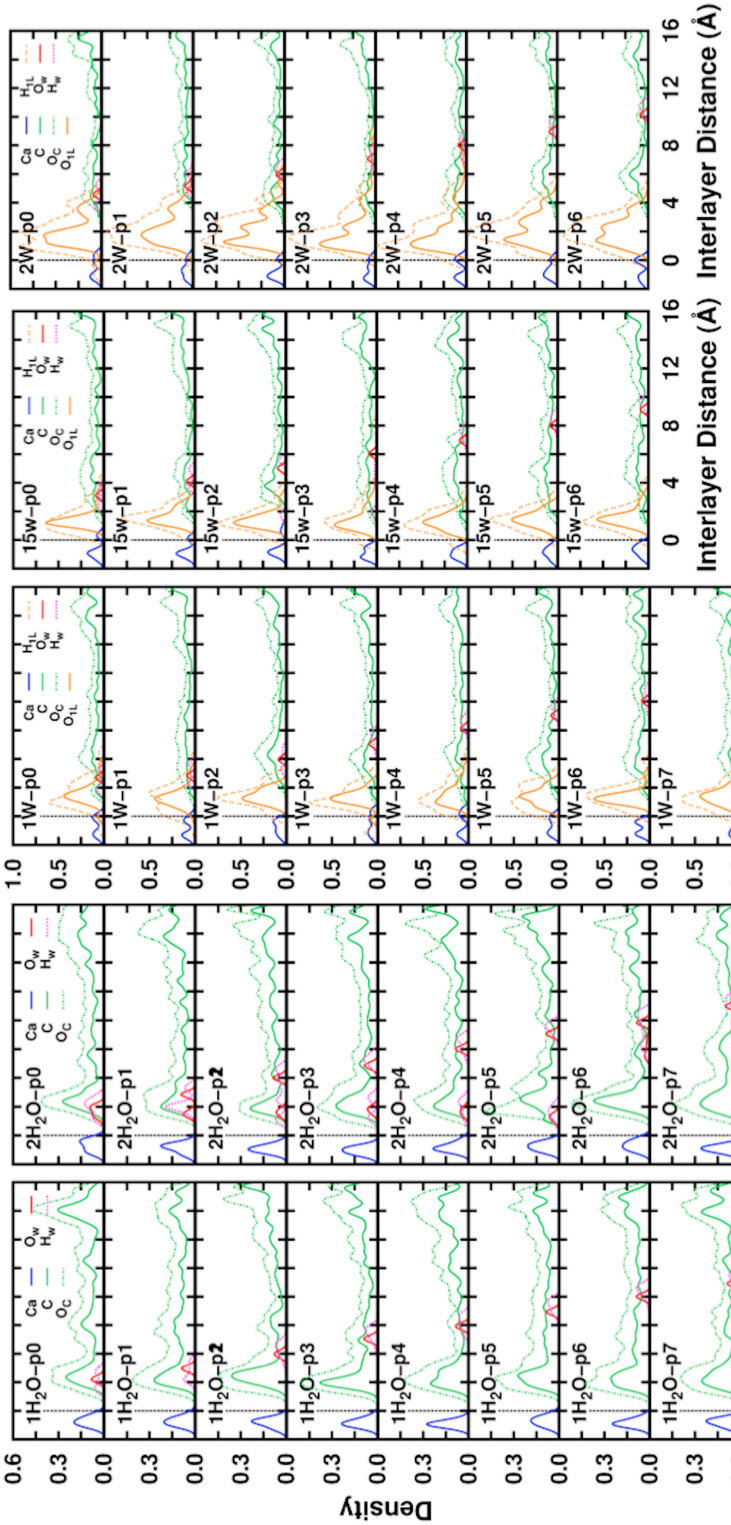

Figure 6. Molecular Density profiles for points along selected PMFs showing how molecular layers are perturbed by the constrained H_2O molecules during the MD. Color Scheme same as Figure 7 in main text.

S6. Converting dimer and timer ΔA to correct reference state.

As discussed in the text the dimer (n=2) and trimer (n=3) simulations are performed with regards to a reference which is different from that of the n=1,7,18 and 14 simulations. We can however adjust the resulting ΔA values by the following arguments:

For the dimer we performed the simulation:

$(H_2O)_2(scCO_2) \rightarrow 2H_2O(ads)$ ΔA=-49 kJ/mol (RS2-1)

To make this consistent with n=7-14 we need to compute:

$H_2O(ads)+H_2O(scCO_2) \rightarrow 2H_2O(ads)$ (RS2-2)

The dimer can be converted to a reference state of two monomers by the following chemical reactions:

$2H_2O(scCO_2) \rightarrow (H_2O)_2(scCO_2)$ ΔA=-1 kJ/mol[3] (RS2-3)

The adsorption of 1 monomer relative to a dimer can be expresses as:

$(H_2O)_2(scCO_2) \rightarrow H_2O(ads)+H_2O(scCO_2)$ ΔA=-33 kJ/mol (RS2-4)

The free energy of (RS2-5) can be obtained by the following relationship (RS2-3)+(RS2-4) = (RS2-5):

$2H_2O(scCO_2) \rightarrow H_2O(ads)+H_2O(scCO_2)$ ΔA=-34 kJ/mol (RS2-5)

which is the reaction for the monomer obtained in the text.

Now subtracting reaction RS2-4 from RS2-1 provides reaction RS2-2. Hence:

$H_2O(ads)+H_2O(scCO_2) \rightarrow 2H_2O(ads)$ ΔA=-15 kJ/mol (RS2-2)

Similarly for the trimer. We have computed:

$(H_2O)_3(scCO_2) \rightarrow 3H_2O(ads)$ ΔA=-50 kJ/mol (RS3-1)

We require:

$2H_2O(ads)+H_2O(scCO_2) \rightarrow 3H_2O(ads)$ (RS3-2)

To achieve this, we note that:

$3H_2O(scCO_2) \rightarrow (H_2O)_3(scCO_2)$ ΔA=-17 kJ/mol[1] (RS3-3)

$(H_2O)_3(scCO_2) \rightarrow H_2O(ads)+2H_2O(scCO_2)$ ΔA=-17 kJ/mol (RS3-4)

The energies of (RS3-4) comes from the use of the monomer reaction (-34 kJ/mol) and reaction (RS3-3). We can rewrite reaction (RS2-2) as reaction (RS3-5):

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[3] Glezakou, V. A.; Rousseau, R.; Dang, L. X.; McGrail, B. P. *Physical Chemistry Chemical Physics* **2010**, *12*, 8759.

$H_2O(ads)+2H_2O(scCO_2) \rightarrow 2H_2O(ads)+H_2O(scCO_2)$ ΔA=-15kJ/mol (RS3-5)

Summing (RS3-3) and (RS3)-5 provides:

$(H_2O)_3(scCO_2) \rightarrow 2H_2O(ads)+H_2O(scCO_2)$ ΔA=-32kJ/mol (RS3-6)

Finally subtracting (RS3-6) from (RS3-1) provides:

$2H_2O(ads)+H_2O(scCO_2) \rightarrow 3H_2O(ads)$ ΔA=-18kJ/mol (RS3-2)

S7. Entropy change using quasiharmonic approximation

To verify the entropy changes estimated from the Blue-Moon ensemble calculations reported in the text, we calculated entropies using a quasi-harmonic approximation where translational, rotational, and vibrational entropies are calculated from the principal root-mean-square fluctuations for the center of mass of H_2O molecule, the principal moments of inertia of a H_2O molecule, and vibrational density of states (VDOS), respectively. Detailed description of this approach can be found in the reference 4[4]. For the translational and rotational entropies, we used unconstrained MD simulation conducted with a configuration with one H_2O molecule in the middle of the interlayer, while the vibrational entropy is calculated using constrained MD simulations conducted at two end positions (with H_2O in the middle of the $scCO_2$ phase and the other with H_2O at the surface). We have chosen two systems with 10 H_2O and 14 H_2O representing significant changes in entropy. The Table below shows the values of $T\Delta S$ obtained using the two independent methods.

System	Blue-Moon method (kJ/mol)	Quasi-harmonic analysis (kJ/mol)
$10H_2O$	-49±3	-60±9
$14H_2O$	-43±2	-52±8

The entropic contribution from translation and rotation is ~40 kJ/mol for both systems. We should point out that convergence of the VDOS calculation is much slower than that for the force calculation. Error analysis of entropy from VDOS shows a larger error (~15 %) than that with Blue-Moon method (~5 %). Thus results from two methods agree fairly well, giving confidence to our discussion about free energetics.

[4] Carlsson, J. and Åqvist, J. *The Journal of Physical Chemistry B* **2005**, 109, 6448-6456.

S8. Cartesian coordinates and cell parameters of structures employed in binding energy analysis.

A. Anorthite slab + 14 H_2O

CRYSTAL
PRIMVEC
16.4340235543 0.0000000000 0.0000000000
-0.3203164176 13.0680953535 0.0000000000
-0.2856096309 0.0038537095 34.9691087411
PRIMCOORD
358 1

Si	6.8850926111	10.6133596982	1.6770133577
Si	15.0910314798	10.6113212861	1.6732846128
Si	4.2289296540	9.8067613651	1.9096187243
Si	12.4545188432	9.8092317653	1.8758843031
Si	6.6438712353	5.5665535246	2.2467199291
Si	14.8769109363	5.5623647355	2.2732292394
Si	12.2467109593	6.8691059977	2.3174123334
Si	3.9994344309	6.8729009176	2.3138754535
Si	0.0880322662	9.8837008947	4.2288309439
Si	8.3354421876	9.8973983655	4.2096410661
Si	8.1630810463	6.7678238120	4.4034399060
Si	-0.0551632076	6.7605124877	4.4543055033
Si	5.3588496266	10.7080718558	4.8643211528
Si	13.5609925195	10.7060111497	4.8576054332
Si	5.1049458112	5.8408238223	4.8777615969
Si	13.3313104521	5.8460610733	4.9093824197
Si	12.2290299909	10.1387781643	7.6567021885
Si	4.0318725598	10.1383950142	7.6629106518
Si	4.1459620368	5.5178351267	7.7709169928
Si	12.3466293699	5.5395869387	7.7865379003
Si	9.3747830075	9.3032920829	8.4269931772
Si	1.1913087224	9.3104627023	8.4488018587
Si	1.1659485691	6.2473811760	8.6171763139
Si	9.3509607811	6.2414767206	8.6130782002
Si	13.5593191630	9.3638265724	10.3452933629
Si	5.3548298709	9.3605287670	10.3497938552
Si	5.2524093489	6.3152876758	10.5861345140
Si	13.4745524107	6.3221694607	10.6153515252
Si	10.5789896146	10.1198520845	11.2153012343
Si	2.3897592362	10.1227709397	11.2525666581
Si	2.4680026404	5.4445644890	11.2666685582
Si	10.6700237820	5.4553388425	11.2579519627
Si	9.2812823226	9.6023380938	14.0057584228
Si	1.0605663343	9.6127726192	14.0249527926
Si	1.1483256849	4.9628288362	14.0906964002
Si	9.4001669658	4.9444155450	14.0853339098
Si	6.4599332422	8.7559434567	14.5510025590
Si	14.6663783325	8.7805282182	14.5941146299
Si	6.3927694156	5.7116280770	14.8453654218
Si	14.6103988873	5.7497172271	14.8168896091
Si	10.4444617787	8.8099273186	16.7023309894
Si	2.2324137480	8.8430109864	16.7605966955

Si	2.2137668712	5.8462331458	16.9088610185
Si	10.5214453233	5.8174156061	16.8632991772
Si	7.4042030039	9.4070690379	17.4819717333
Si	15.6355389167	9.4023741758	17.5521794199
Si	15.8013714062	5.0173378980	17.5945382325
Si	7.6300118682	4.9883511689	17.5976201616
Al	8.4648782759	3.2771297128	1.5829864263
Al	0.2756383911	3.2818928293	1.5650381895
Al	2.9322290340	12.4985940180	1.6087722071
Al	11.1175181803	12.4925221123	1.6016238861
Al	10.8605789873	4.1160992806	1.7493815210
Al	2.6675430574	4.1107418207	1.7491103973
Al	8.3542966216	0.3005735115	2.2045466298
Al	0.1568864359	0.3100363416	2.1897964874
Al	13.0750310181	3.3693304829	3.6784418168
Al	4.8526370203	3.3538260950	3.6862296907
Al	12.7276558008	0.4737027280	4.0600851567
Al	4.5070500491	0.4600857325	4.0770765312
Al	10.1276573254	4.3166248589	4.7041297302
Al	1.9262155567	4.3136739930	4.7013141320
Al	9.4298560208	12.5427766579	4.8954170484
Al	1.1772568173	12.5392867922	4.8755781433
Al	8.5832425537	3.5237873500	7.4913470666
Al	0.3715694003	3.5378979112	7.4840234208
Al	-0.0838584020	12.0089551888	7.8316073872
Al	8.1111681065	12.0059445333	7.8221240342
Al	5.5619699556	2.7703903122	8.1967849108
Al	13.7969311820	2.8052813591	8.2259018350
Al	5.0453756229	12.8370728134	8.4266493987
Al	13.2735657088	12.8471361798	8.4752157872
Al	1.6206618153	2.8234728884	10.3291446512
Al	9.8186536990	2.8236586407	10.3331703296
Al	1.1001084045	12.8532076769	10.8270245922
Al	9.3010686544	12.8512089263	10.8252978204
Al	6.7995012501	3.5490681822	11.1564995338
Al	15.0453158942	3.5648176891	11.2002040568
Al	14.5273427524	12.1268450741	11.3411844308
Al	6.3158729696	12.1273291469	11.2933927649
Al	5.3279321330	2.9799841509	13.9915143876
Al	13.5854722949	2.9656099445	14.0430415264
Al	4.9337381368	11.4818982833	14.1188821672
Al	13.1680336415	11.5218554208	14.2133737689
Al	2.3885635671	2.1638223361	14.6583654739
Al	10.6301726818	2.1715570121	14.6298647495
Al	1.8761584276	12.1983217978	14.9493821681
Al	10.0716128005	12.2077345533	15.1355445578
Al	6.6120783685	2.2201946989	16.8677090749
Al	14.9628569710	2.2148686951	16.9045126398
Al	6.2069137471	12.2537816542	17.0220636188
Al	14.4728207193	12.2680225152	17.1078840738
Al	3.4845819578	3.1500394864	17.6713471430
Al	11.8295368530	3.1696111570	17.6590031598
Al	3.1465199863	11.6252579578	17.7826885495

Al	11.3877334180	11.5601691307	17.8416583472
O	9.7787665930	3.6185146754	0.5212278210
O	1.5945819130	3.6220872238	0.5136024199
O	13.9183121349	9.7276402551	1.0381451971
O	5.7006780559	9.7151153855	1.0951443751
O	11.4232767241	10.8185454975	1.2347575155
O	3.2329929011	10.8263207743	1.2350990007
O	7.1320191750	4.4314528719	1.3126440955
O	15.3768497806	4.4414487772	1.3266610548
O	1.6663814111	-0.1335651597	1.4706891439
O	9.8524548565	-0.1352729082	1.4606168679
O	6.9278103749	12.1203648978	1.3839106515
O	15.1764341772	12.1159907899	1.3819714241
O	15.9226316216	1.8273972838	1.9049434812
O	7.6786310929	1.8286959233	1.9774137968
O	5.4650917686	6.5368021393	1.6763347986
O	13.7096244823	6.5326382302	1.6784555082
O	3.5098109583	8.3636772347	1.9002652271
O	11.7579142063	8.3582147325	1.8973088900
O	11.0803253898	5.8690412767	2.0368322559
O	2.8355108339	5.8695560930	2.0351008588
O	12.3258034715	3.3341878867	2.1830802274
O	4.1368096205	3.3334500333	2.1763935396
O	12.7570308948	0.0671195286	2.4041874035
O	4.5727800330	0.0718532171	2.4134128159
O	-0.3365292231	9.8012298053	2.6305932526
O	7.9178612796	9.8112503099	2.6114639344
O	7.8469191093	6.5386145119	2.8430144921
O	-0.3895765146	6.5495278966	2.8992765750
O	9.6076194750	3.7956596980	3.1261663455
O	1.4171690650	3.7832811865	3.1242991667
O	13.0181062999	10.0961719756	3.4384546137
O	4.7521833071	10.0884436010	3.4827292942
O	14.2340410433	4.8672102489	3.7644675125
O	5.9914978135	4.8682680215	3.7287741160
O	8.3516565385	-0.1449427334	3.9318567006
O	0.1091306504	-0.0852598778	3.9283480583
O	12.5722887248	7.0498883688	4.0049210822
O	4.3220436142	7.0483500912	4.0020133861
O	1.3725249261	10.7459232501	4.5967815340
O	9.6261515257	10.7452316200	4.6024972713
O	8.7378366516	8.3406307153	4.6757985343
O	0.4899852881	8.3409352132	4.7384354677
O	13.5737886825	1.9539007063	4.5237398791
O	5.3197069597	1.9537141615	4.5779945900
O	11.1921454748	0.4324535152	4.8730000090
O	2.9639454897	0.3756850696	4.8680122364
O	5.2069354467	12.2734587463	4.9569477048
O	13.3933180958	12.2706172660	4.9598671483
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B. Anorthite slab + 9 CO_2

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